Solving Stefan problem through C-NEM and level-set approach

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Introduction

Final goal of the study

Develop numerical time domain approach able to simulate thermo-mechanical phenomena in Finite Transformations:

- Cutting/blanking processes in 3D
  - Matter splitting encountered in forming processes
- Laser drilling/cutting
  - Multi-phases problem with moving interfaces across the matter
- **Research tool** in order to be able to test new approaches and thermomechanical models

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The approach must handle:

- Large strains
- Contact
- Interfaces and discontinuities

Introduction

Large strains

- FEM: induced **mesh distorsions** are conducting to frequent re-meshing and fields projections
  - need a very efficient mesher → lack of robustness in 3D
- **Mesh Free**: only the distribution and number of nodes are to be managed
  - OK but need to simply take into account boundary conditions

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Large strains

- FEM: induced **mesh distorsions** are conducting to frequent re-meshing and fields projections
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- **Mesh Free**: only the distribution and number of nodes are to be managed
  - OK but need to simply take into account boundary conditions

Mesh Free

We have choose to use a Natural Neighbor interpolant based mesh free approach $\Rightarrow$ nodal interpolation

Existing methods:

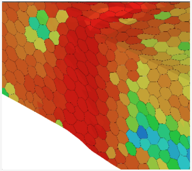
- α-NEM[1]: no geometrical description of the boundaries **but** boundaries must be quite regular
- C-Nem[2,3]: a geometrical model is needed for the boundaries **but** domain can be highly non convex

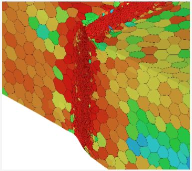
[1] E. Cueto, Int. J. Numer. Meth. in Engng, 2000
[2] J. Yvonnet, Int. J. Numer. Meth. in Engng, 2004 [3] L. Illoul, Comp. and Struc., 2011

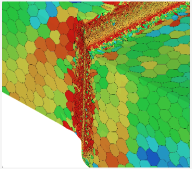
Introduction

Interfaces and discontinuities

Example of blanking process: (C-Nem simulation[1])





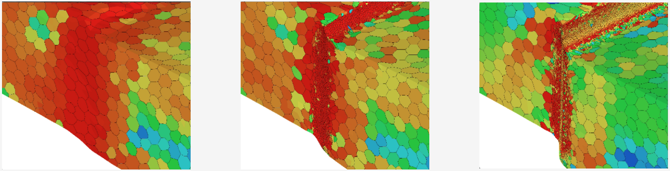


1 L. Illoul, http://sn-m2p.cnrs.fr

Introduction

Interfaces and discontinuities

Example of blanking process: (C-Nem simulation[1])



[1] L. Illoul, http://sn-m2p.cnrs.fr

Interfaces modeling

- Full geometrical model: in 3D the shape evolution of the interface need a complex (and robust) surface mesher
  - Discontinuities: direct with duplication of the variables on nodes belonging to the interface[2]
- **Level-set**: easy but the description is linked to the nodes distribution
  - Discontinuities: X-FEM framework → **X-NEM**[3]

[2] J. Yvonnet, Int. J. Therm., 2005
[3] N. Sukumar, U.S. National Congress on Comp. Mech., 2001

Introduction

Goals of the presentation

Present a numerical method to solve problems involving discontinuities on moving internal boundaries with:

- a C-Nem approach for the interpolation (based on the natural neighbours interpolation)
- a level-set technique to represent the interface
- a local enrichement through the partition of unity concept

First results in 2D for the Stefan problem are presented

Outline

Few words on the C-Nem

C-Nem use a Ritz(-Galerkin) approach

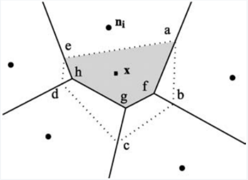
$$\boldsymbol{u}^h(\boldsymbol{x}) = \sum_{i=1}^{n} N_i(\boldsymbol{x})\boldsymbol{u}_i, \qquad \forall \boldsymbol{x} \in \Omega$$

where $N_i(\boldsymbol{x})$ are **Natural Neighbour (NN) shape functions**: one shape function per node i

Natural Neighbour shape function

Based on :

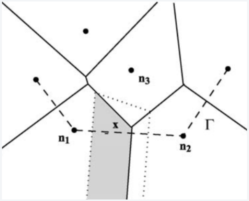
- Voronoï diagram ⇔ Delaunay tessellation
- Systematic geometric constructions (for a given set of nodes)



$\boldsymbol{x}$ inside Ω

Sibson shape function

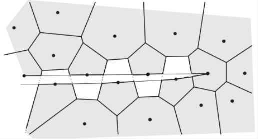
$$N_i(\boldsymbol{x}) = \frac{\text{Area(afghe)}}{\text{Area(abcde)}}$$



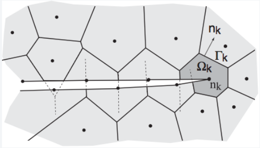
$\boldsymbol{x}$ on the boundary of Ω

Few words on the C-Nem

Natural Neighbour (NN) shape function – Non-convex domains

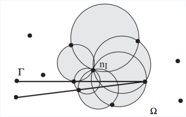


Voronoï diagram with NN

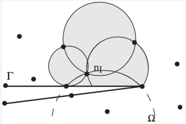


Constrained Voronoï diagram with NN

The constrained Voronov diagram (Delaunay tessellation) use a visibility criterion.
The Delaunay tessellation is **constrained** to respect the tessellation of $\partial\Omega$



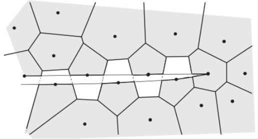
NN supports



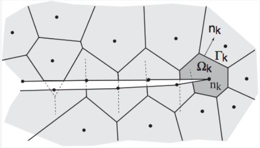
Constrained NN supports

Few words on the C-Nem

Natural Neighbour (NN) shape function – Non-convex domains



Voronoï diagram with NN



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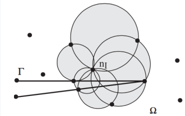
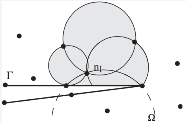


NN supports



Constrained NN supports

C-Nem: Constrained Natural Element Method

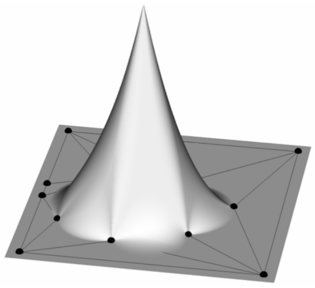
C-NEM use the constrained NN shape functions

Few words on the C-Nem

Properties of (constrained) NN interpolant

- Delta Kronecker:
  $N_i(\boldsymbol{x}_j) = \delta_{ij}$
- Positivity:
  $0 \leq N_i(\boldsymbol{x}) \leq 0$
- **Partition of unity**:
  $\sum_{i=1}^{n} N_i(\boldsymbol{x}) = 1$
- Local coordinate property:
  $\boldsymbol{x} = \sum_{i=1}^{n} N_i(\boldsymbol{x})\boldsymbol{x}_i$
  $\Rightarrow$ exact interpolation of linear fields
  $\Rightarrow$ reproduction of large solid motions

A Sibson shape function



Continuity

Natural neighbor shape functions are C^∞ at any point except :

- at the nodes: C^0
- on the boundary of the Delaunay circles (spheres in 3D): C^1

Outline

Coupling C-Nem with a level-set approach

Main aspects

We propose to use a X-FEM like strategy by enriching the C-Nem approximation space through the **partition of unity technique**.

As for the X-FEM, the **location of the discontinuity interface** is defined by a **level-set function**. This latter being defined by the nodal values of the level-set function with the **C-Nem approximation**.

We need to define :

- the adequate enrichment function (depending on the discontinuity), based on the level-set (distance) function
- the selection of the nodes subjected to enrichment (near the interface)
- the quadrature rules for the weak forms

Coupling C-Nem with a level-set approach

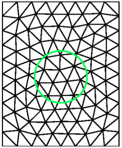
Local enrichment of the Constrained NN interpolant

$$T^h(\mathbf{x},t) = \sum_i N_i(\mathbf{x}) a_i(t) + \sum_{j \in I(t)} \underbrace{N_j(\mathbf{x}) \psi(\mathbf{x},t)}_{M_j(\mathbf{x},t)} b_j(t)$$

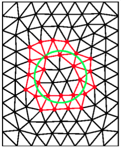
- $\psi(\mathbf{x},t)$ is the enrichment function depending on the interface position
- $I(t)$ is the set of the nodes subjected to enrichment
- $N_i(\boldsymbol{x})$ are the Constrained NN shape function verifying the partition of unity. If the geometry of the domain do not evolve, these shape functions do not depend on time.

Selection of the nodes subjected to enrichment

In order to define the set $I(t)$ we use the constrained Delaunay tessellation.



Constrain Delaunay Tesselation (black) + Discontinuity interface (green)



Enriched nodes selection (in red)

Coupling C-Nem with a level-set approach

Enrichment function ψ

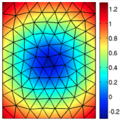
Here we have chosen a enrichment function, proposed by Moes et al[1], in order handle weak discontinuity (gradient discontinuity) :

$$\psi(\mathbf{x},t) = \sum_{j \in I(t)} N_j(\mathbf{x}) \left|\Phi(\mathbf{x}_j,t)\right| - \left|\sum_j N_j(\mathbf{x}) \Phi(\mathbf{x}_j,t)\right|$$

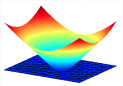
where $\Phi(\mathbf{x}_j,t)$ is the level-set (distance) function

[1] N. Moes, Comput. Methods Appl. Mech. Engrg, 2003

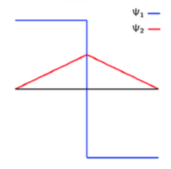
Representation of the level-set and enrichment functions



$\Phi(\mathbf{x})$: Level-set contours



$\Phi(\mathbf{x})$: Level-set contours in 3D

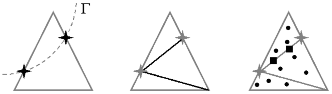


$\psi(\mathbf{x})$: Schematic representation

Coupling C-Nem with a level-set approach

Quadrature

- For the **integration** of the **weak forms** we use the **constrained Delaunay tessellation**
- As for the X-Fem, the triangles (tetrahedrons in 3D) intersecting the interface, are re-meshed in order to be **compatible with the interface** and to **improve the quadrature**.

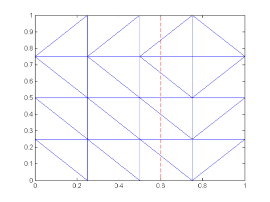


✦ Intersecting points

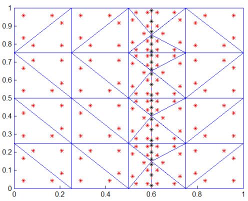
● Surface (volume in 3D) quadrature points

■ Line (surface in 3D) quadrature points

Example of quadrature points distribution



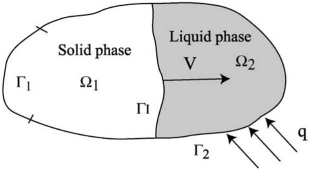
Initial Delaunay mesh



Refined Delaunay mesh – Quadrature points

Outline

Stefan problem



Strong form

- Heat equation :

  $\rho \frac{\partial}{\partial t}(c_1 T) = \nabla \cdot (k_1 \nabla T)$ in $\Omega_1(t)$; $\rho \frac{\partial}{\partial t}(c_2 T) = \nabla \cdot (k_2 \nabla T)$ in $\Omega_2(t)$

  c_i, k_i : heat capacities, thermal conductivities $\rho = \rho_1 = \rho_2$: density

- Initial and boundary conditions :

$$\begin{cases} T(\boldsymbol{x}, t=0) = T_0 & \forall \boldsymbol{x} \in \Omega \\ T(\boldsymbol{x}, t) = \overline{T}(\boldsymbol{x}, t) & \forall \boldsymbol{x} \in \Gamma_1, \forall i \in [0, t_{\text{max}}] \\ -k_i \nabla T(\boldsymbol{x}, t) \cdot \boldsymbol{n}_{12} = \overline{q}(\boldsymbol{x}, t) & \forall \boldsymbol{x} \in \Gamma_1, \forall i \in [0, t_{\text{max}}] \end{cases}$$

- Interface velocity: depends on L the latent heat of fusion

  $\boldsymbol{V}(\boldsymbol{x} \in \Gamma_I(t)) = \frac{[q]}{L} \boldsymbol{n}_{12}(\boldsymbol{x})$ where $[q] = (k_1 \nabla T|_{\Gamma_{12}^-(t)} - k_2 \nabla T|_{\Gamma_{12}^+(t)}) \cdot \boldsymbol{n}_{12}$

- Constraint prescribed on the interface $\Gamma_I(t)$:
  $T(\boldsymbol{x}, t) = T_m$ $\forall \boldsymbol{x} \in \Gamma_I(t)$; T_m: melting temperature

Stefan problem

Weak form

Find $T \in H^1(\Omega)$ with $T = \bar{T}$ on Γ_1 such that

$$\int_\Omega \rho c \frac{\partial T}{\partial t} \delta T \, d\Omega + \int_\Omega k \, \nabla T \cdot \nabla \delta T \, d\Omega = \int_{\Gamma_I} \alpha \left(T - T_m\right) \delta T d\Gamma + \int_{\Gamma_I} [\![\mathbf{q} \cdot \mathbf{n}_{12}]\!] \, \delta T d\Gamma$$

(Simplify form : $\overline{q}(t) = 0$)

Time discretization using implicit scheme 1

The implicit backward Euler integration scheme between t^{n-1} and t^n gives:

$$\int_\Omega \rho c \frac{T^n - T^{n-1}}{dt} \delta T^n \, d\Omega + \int_\Omega k \, \nabla T^n \cdot \nabla \delta T^n \, d\Omega = \int_{\Gamma_I} \alpha \left(T^n - T_m\right) \delta T^n d\Gamma + \int_{\Gamma_I} [\![\mathbf{q}^n \cdot \mathbf{n}_{12}^n]\!] \, \delta T^n d\Gamma$$

Stefan problem

Time discretization using implicit scheme 1

$$\int_\Omega \rho c \frac{T^n - T^{n-1}}{dt} \delta T^n \, d\Omega + \int_\Omega k \, \nabla T^n \cdot \nabla \delta T^n \, d\Omega = \int_{\Gamma_I} \alpha \left(T^n - T_m\right) \delta T^n d\Gamma + \int_{\Gamma_I} [[\mathbf{q}^n \cdot \mathbf{n}_{12}^n]] \, \delta T^n d\Gamma$$

Time discretization using implicit scheme 2

$$\int_\Omega \rho c T^n \delta T^n \, d\Omega + dt \int_\Omega k \, \nabla T^n \cdot \nabla \delta T^n \, d\Omega = \int_\Omega \rho c T^{n-1} \delta T^n \, d\Omega + dt \int_{\Gamma_I} \alpha \left(T^n - T_m\right) \delta T^n d\Gamma + dt \int_{\Gamma_I} (k_1 - k_2) \left(\nabla T^n \cdot \mathbf{n}_{12}^n\right) \delta T^n d\Gamma$$

Stefan problem

Time discretization using implicit scheme 2

$$\int_\Omega \rho c T^n \delta T^n \, d\Omega + dt \int_\Omega k \, \nabla T^n \cdot \nabla \delta T^n \, d\Omega = \int_\Omega \rho c T^{n-1} \delta T^n \, d\Omega$$
$$+ \, dt \int_{\Gamma_I} \alpha \left(T^n - T_m\right) \delta T^n d\Gamma + dt \int_{\Gamma_I} \left(k_1 - k_2\right) \left(\nabla T^n \cdot \mathbf{n}_{12}^n\right) \delta T^n d\Gamma$$

Matrix Form

$$\left(\mathbf{C} + dt\mathbf{K}\right) \mathbf{T}^n = \mathbf{F}$$

with

$$\mathbf{C} = \int_\Omega \rho c \mathbf{N}^{nT} \mathbf{N}^n \, d\Omega$$
$$\mathbf{K} = \int_\Omega k \, \mathbf{B}^{nT} \mathbf{B}^n \, d\Omega - \int_{\Gamma_I} \alpha \mathbf{N}^{nT} \mathbf{N}^n d\Gamma + \int_{\Gamma_I} \left(k_2 - k_1\right) \mathbf{N}^{nT} \left(\mathbf{B}^n \cdot \mathbf{n}_{12}^n\right) d\Gamma$$
$$\mathbf{F} = \int_\Omega \rho c \mathbf{N}^{nT} \left(\mathbf{N}^{n-1} \mathbf{T}^{n-1}\right) \, d\Omega + dt \int_{\Gamma_I} \left(\alpha \, T_m\right) \mathbf{N}^{nT} d\Gamma$$

Stefan problem

Interface convection[1]

Velocity extension

$$\text{sign}(\Phi)\nabla F \cdot \nabla \Phi = 0 \qquad \text{with } F = \mathbf{V} \cdot \boldsymbol{n}_{12} \text{ on } \Gamma_I$$

Level-set updating

$$\frac{\partial \Phi}{\partial t} + \mathbf{V} \cdot \nabla \Phi = 0$$

[1] J. Chessa, Int. J. Numer. Meth. Engng, 2002

Stefan problem

Pseudo-code

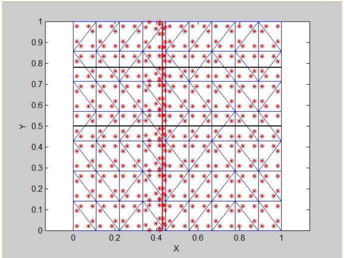
Let $\mathbf{T}^{n-1}$ and Φ^{n-1} be known.

- Compute the velocity of the interface $\mathbf{V}^{n-1}$ on Γ_I
  $\mathbf{V}^{n-1} = \frac{[\mathbf{q}]}{L} \boldsymbol{n}_{12}^{n-1}$
- Extend this velocity to the whole domain Ω solving
  $\text{sign}(\Phi) \nabla F \cdot \nabla \Phi = 0$ with $F = \mathbf{V}^{n-1} \cdot \mathbf{n}_{12}$ on Γ_I
- Determine Φ^n by updating the level-set function through
  $\frac{\partial \Phi}{\partial t} + F \, |\nabla \Phi| = 0$
- Localize integration points by dividing the elements cut by Γ_I into sub-elements matching Γ_I using Φ^n only
- Build matrices $\mathbf{C}$ & $\mathbf{K}$ and vector $\mathbf{F}$
- Compute $\mathbf{T}^n$ by solving the heat equation
  $(\mathbf{C} + dt\mathbf{K})\, \mathbf{T}^n = \mathbf{F}$

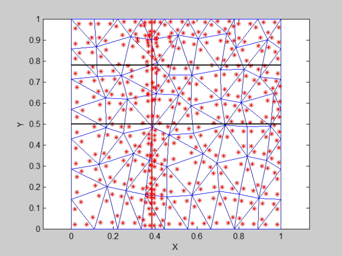
Outline

First results

Motion on the interface across the mesh



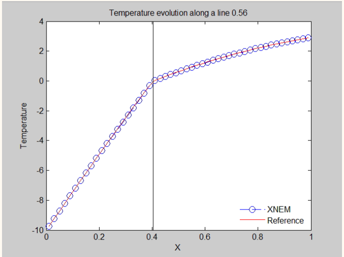
Regular grid



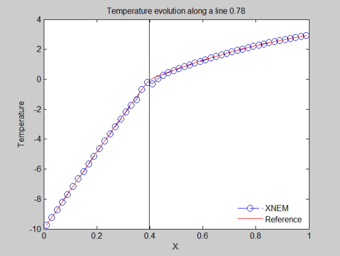
Irregular grid

First results

Motion of the interface at two Y levels



Level $Y = 0.56$

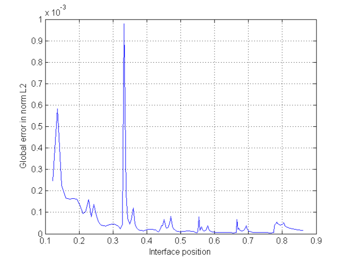


Level $Y = 0.78$

First results

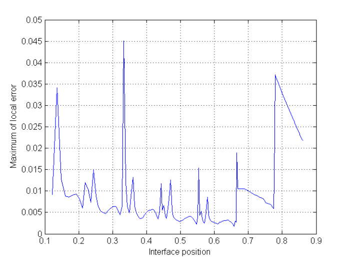
Global and local errors on temperature

Global error



$$e^2(t) = \int_{\Omega(t)} \frac{[T_{Num}(\boldsymbol{x},t) - T_{Sol}(\boldsymbol{x},t)]^2}{[T_{Sol}(\boldsymbol{x},t)]^2} \mathrm{d}S$$

Local error



$$e(t) = \sup_{\boldsymbol{x}\in\Omega} \frac{|T_{Num}(\boldsymbol{x},t) - T_{Sol}(\boldsymbol{x},t)|}{|T_{right} - T_{left}|}$$

Outline

Conclusion

Weak form

- First results are encouraging
- Partition of unity technique seems to work as well with the C-Nem than with the FEM
- It is a first approach in 2D, investigation must be done on more complex geometries and in 3D
- Main errors are observed in the "enriched zones" where partition of unity not exactly respected are observed (error $\approx 10^{-2}$)

Work still in progress ...

Thanks for your attention

Any questions ?

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